

A Surface Phase Diagram of Water

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Systematic computer simulations of the liquid-vapor coexistence curves of water in model pores with various sizes and strengths of water-surface interaction, U_0 , allowed us to construct the first surface phase diagram of water. Such a phase diagram reflects the evolution of the liquid-vapor phase transition near a surface with interaction strength U_0 . It indicates the water-surface interaction threshold value, necessary for the appearance of a layering or prewetting transition, which is a quasi-2D condensation of one or two dense water layers on the pore wall, respectively. Also, it shows the variation of the critical temperatures of these transitions and the wetting temperatures with U_0 . In particular, at room temperature, there are no surface transitions, when $U_0 > -3$ kcal/mol; the condensation of two water layers (a prewetting transition) occurs, when U_0 varies between about -3 and -4 kcal/mol; and if $U_0 < -4$ kcal/mol, the condensation of the first water layer occurs via a layering transition, whereas the second layer grows continuously. The effect of confinement on the surface phase diagram is studied. The density profiles of all possible water phases near the surface, and their temperature evolution are analyzed based on theories of the surface phase transitions and surface critical behavior.

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